GEOS-Chem as part of GMI

GEOS-Chem

- Research CTM with large user base (27 institutions in 9 countries) committed to NASA science objectives
- Grass-roots model development
- Management at Harvard directed at
  - code integrity and trackability
  - fast infusion of new developments
  - easy access to code for all
  - user support & participation

↔

GMI

- tropospheric composition modules
- meteorological fields
- software tools (ESMF)

GEOS-Chem support staff at Harvard:

- Bob Yantosca (software engineer)
- Philippe LeSager (research associate)
- Jack Yatteau (systems manager)

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SIVO support staff at GSFC:

- Tom Clune
- Brice Wormack
- Megan Damon

3rd GEOS-Chem Users' Meeting will be held at Harvard on April 11-13, 2007

CURRENT GEOS-Chem CAPABILITIES

- GEOS global assimilated meteorological data, 1983-present; GISS GCM 3 meteorological data
- Resolution: $1^o x 1^o$-$4^o x 5^o$ horizontal, 20-72 layers in vertical, nested capability, linkage to CMAQ regional model
- Open-MP parallelization
- Model adjoint for inverse analyses

Mature applications (in standard model):

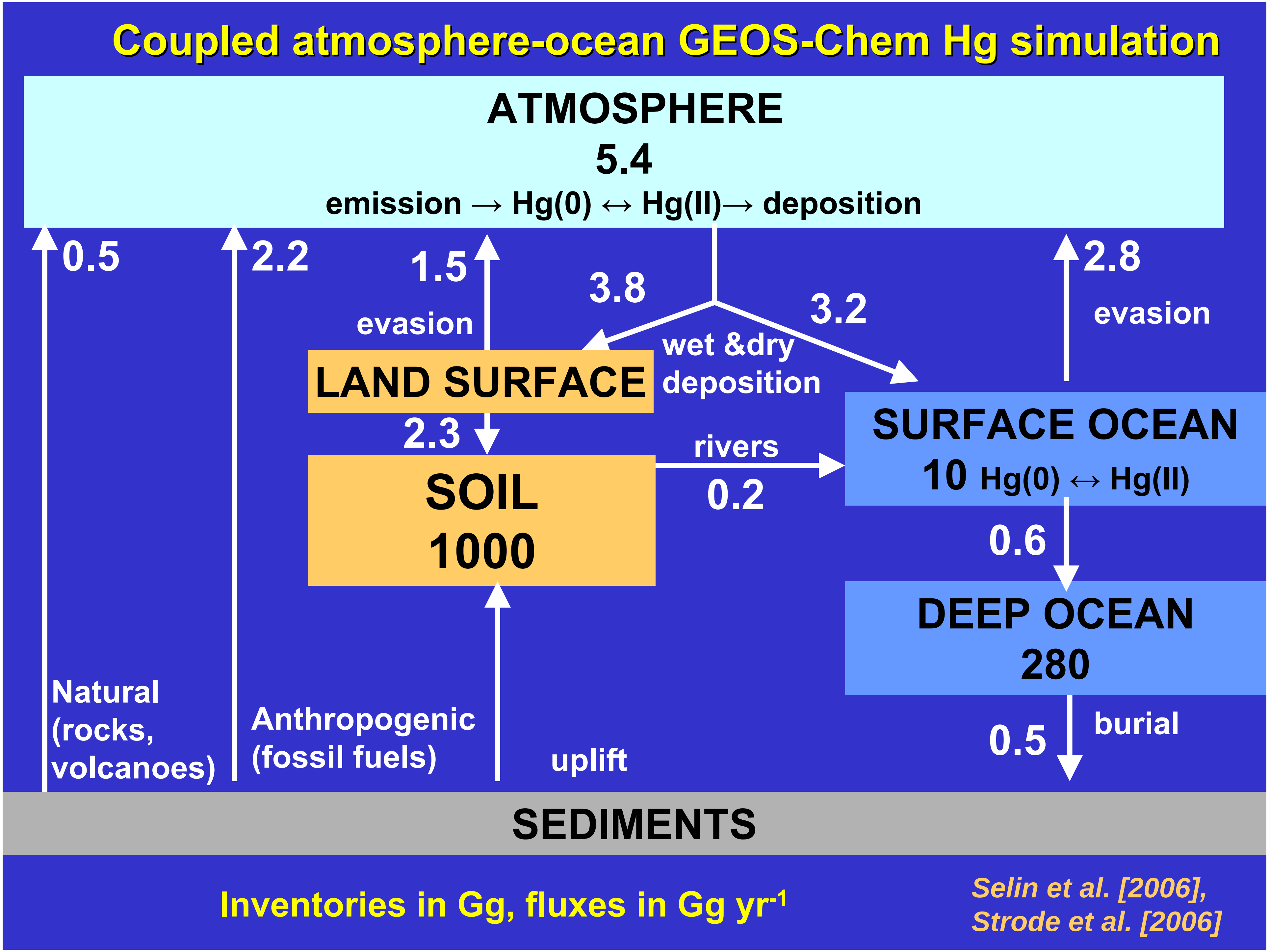
- *Tropospheric ozone and aerosol chemistry*
- *CO_2, CH_4*
- *Mercury*
- *Exotics: oxygenated organics, nitriles, methyl halides, isotopes…*

Under construction:

- *MPI parallelization (JPL)*
- *Aerosol microphysics (CMU, SUNYA)*
- *Aerosol phase transitions (Harvard)*
- *Hydrogen (UW, Duke)*
- *Halogen chemistry (Harvard, U. Leeds, Georgia Tech)*
- *POPs (CSIC-Barcelona)*

New standard GEOS-Chem capabilities available for delivery to GMI

1. **New simulation:**
   - mercury [Selin et al., 2006; Strode et al., 2006; Holmes et al., 2006]
2. **New chemistry:**
   - N_2O_5 reactive uptake [Evans and Jacob, 2005]
   - Secondary organic aerosol formation including isoprene [Henze and Seinfeld, 2006]
3. **New emissions:**
   - MEGAN biogenic VOC inventory [Guenther et al., 2006]
   - EDGAR 2000 anthropogenic emissions inventory
   - Regional anthropogenic inventories; NEI99 for U.S., BRAVO for Mexico, EMEP for Europe, Streets et al. for East Asia
   - GFED2 inventory for biomass burning



Coupled atmosphere-ocean GEOS-Chem Hg simulation
ATMOSPHERE
5.4
emission → Hg(0) ↔ Hg(II)→ deposition
0.5
2.2
1.5
evasion
3.8
3.2
wet &dry
deposition
2.8
evasion
LAND SURFACE
2.3
SOIL
1000
rivers
0.2
SURFACE OCEAN
10 Hg(0) ↔ Hg(II)
0.6
DEEP OCEAN
280
burial
0.5
Natural
(rocks,
volcanoes)
Anthropogenic
(fossil fuels)
uplift
SEDIMENTS
Inventories in Gg, fluxes in Gg yr-1
Selin et al. [2006],
Strode et al. [2006]

Dependence of N_2O_5 reactive uptake on aerosol composition

GEOPHYSICAL RESEARCH LETTERS, VOL. 32, L09813, doi:10.1029/2005GL022469, 2005

Impact of new laboratory studies of N_2O_5 hydrolysis on global model budgets of tropospheric nitrogen oxides, ozone, and OH

M. J. Evans[1] and D. J. Jacob
Division of Engineering and Applied Science, Harvard University, Cambridge, Massachusetts, USA

Table 1. GEOS-CHEM Representation of the Reaction Probability γ_{N2O5} for N_2O_5 Hydrolysis on Aerosol Surfaces

Aerosol Type	Reaction Probability[a]	Reference
Sulfate[b]	$\gamma = \alpha \times 10^{\beta}$	*Kane et al.* [2001]
	$\alpha = 2.79 \times 10^{-4} + 1.3$ $\times 10^{-4} \times RH - 3.43$ $\times 10^{-6} \times RH^2 + 7.52$ $\times 10^{-8} \times RH^3$	
	$\beta = 4 \times 10^{-2}$ $\times (T\text{-}294)\ (T \geq 282K)$	*Hallquist et al.* [2003][c]
	$\beta = -0.48\ (T < 282K)$	
Organic carbon	$\gamma = RH \times 5.2$ $\times 10^{-4}\ (RH < 57\%)$	*Thornton et al.* [2003][d]
	$\gamma = 0.03\ (RH \geq 57\%)$	
Black carbon	$\gamma = 0.005$	*Sander et al.* [2003]
Sea salt	$\gamma = 0.005\ (RH < 62\%)$	*Sander et al.* [2003][e]
	$\gamma = 0.03\ (RH \geq 62\%)$	
Dust	$\gamma = 0.01$	*Bauer et al.* [2004][f]

Global mean
$\gamma = 0.02$

…also shut off HO_2 reactive uptake (Joel Thornton's work)

SOA formation from isoprene

GEOPHYSICAL RESEARCH LETTERS, VOL. 33, L09812, doi:10.1029/2006GL025976, 2006

Global secondary organic aerosol from isoprene oxidation

Daven K. Henze[1] and John H. Seinfeld[1]

Table 1. Stoichiometric Coefficients, α_i, and Equilibrium Partitioning Coefficients, K_i, for SOA Formation From Low NO_x Chamber Experiments of Reaction of Isoprene With OH[a]

Product	α_i	K_i, $m^3\ \mu g^{-1}$ [b]
1	0.232	0.00862
2	0.0288	1.62

[a]See *Kroll et al.* [2006].
[b]Reference temperature is 295 K.

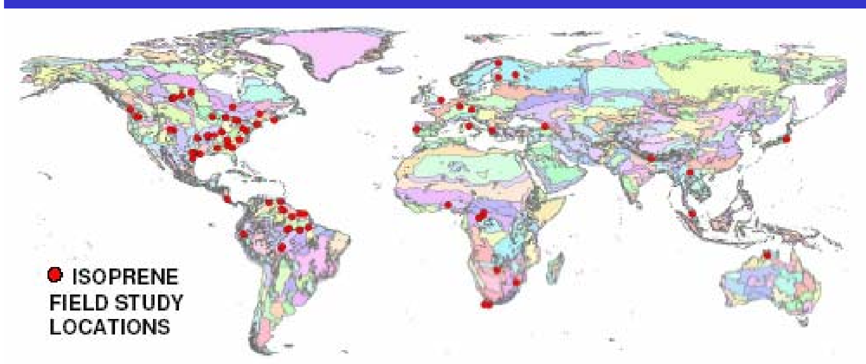
MEGAN EMISSION INVENTORY FOR BIOGENIC VOCs

Atmos. Chem. Phys., 6, 3181–3210, 2006
www.atmos-chem-phys.net/6/3181/2006/

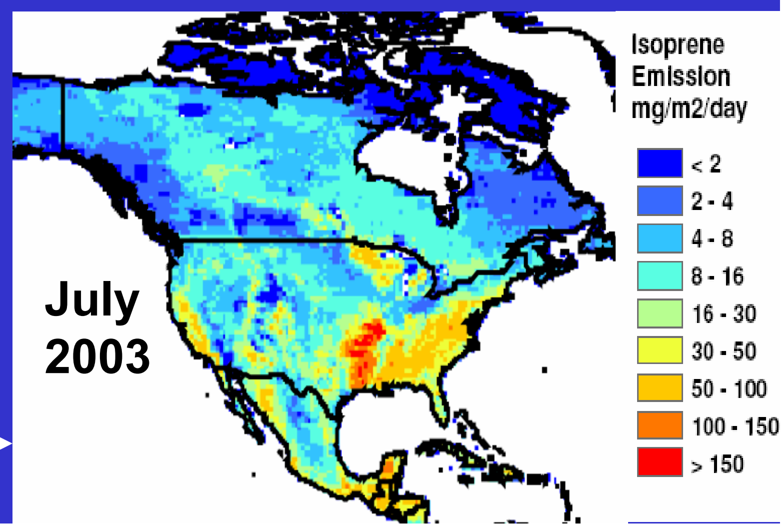
Atmospheric Chemistry and Physics

Estimates of global terrestrial isoprene emissions using MEGAN (Model of Emissions of Gases and Aerosols from Nature)

A. Guenther[1], T. Karl[1], P. Harley[1], C. Wiedinmyer[1], P. I. Palmer[2], and C. Geron[3]



Environmental factors:
- temperature
- solar irradiance
- leaf area index
- leaf age



Anthropogenic Emissions Update

- GEOS-Chem emissions use 1985 as a base year
- These are projected forward using national inventories (U.S., Europe, Japan, etc) and national fossil fuel use from CDIAC
- The projection uses the same spatial distribution within a country
- 20 years is a long time to project forward!

- EDGAR 2000 is now an option in GEOS-Chem.

  (It is based on their 1995 inventory and updated fuel statistics)
- EDGAR 2000 has known flaws

Options to overwrite EDGAR 2000

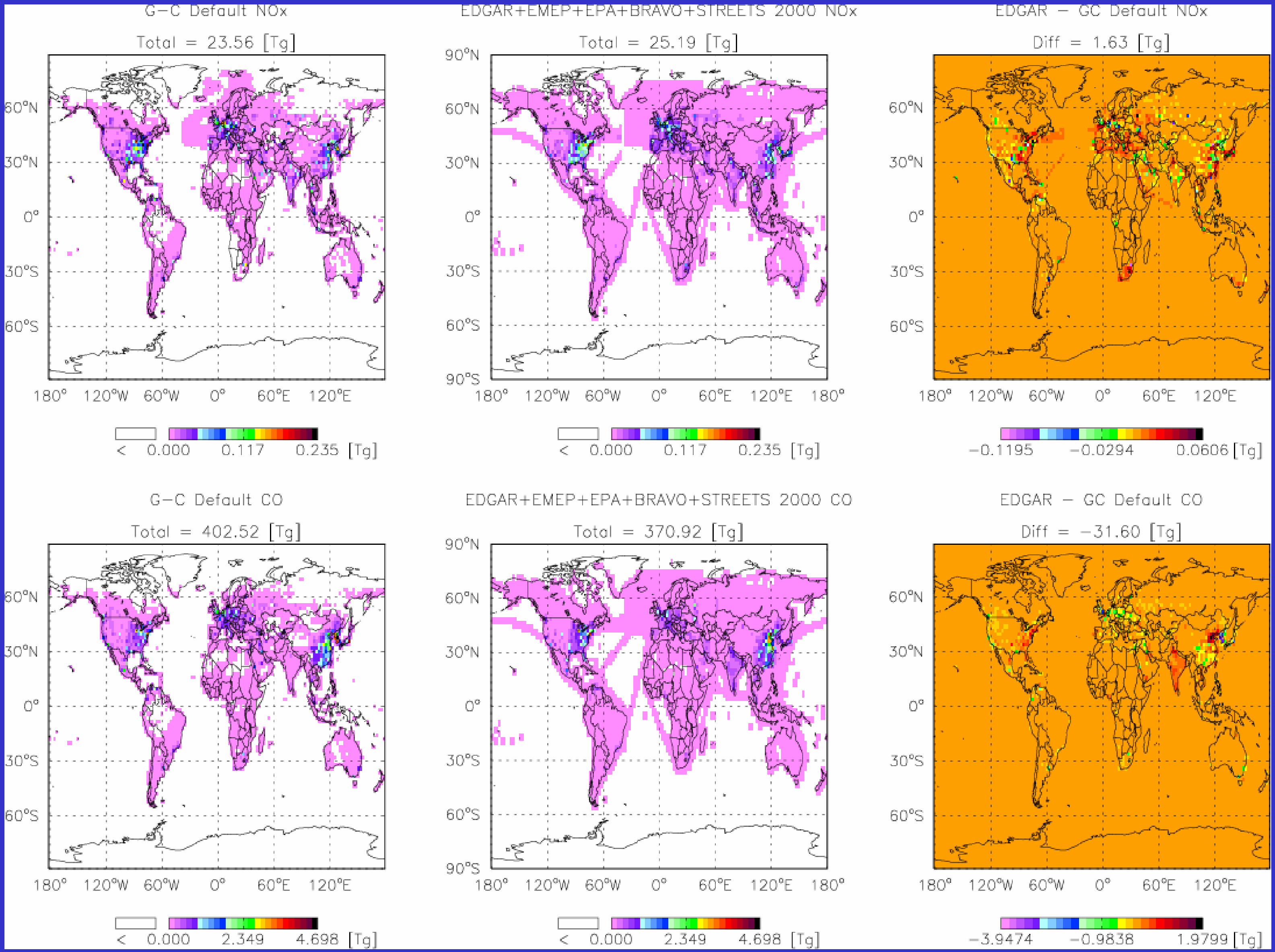
- These options are important particularly for CO, for which EDGAR is known to be much too low in Asia.

- EPA, NEI-99 for the U.S.
- EMEP for Europe
- Streets et al. [2006] for China, 2001 (updated TRACE-P)
- Streets et al. [2003], TRACE-P, 2000, for the rest of Asia
- BRAVO for Mexico

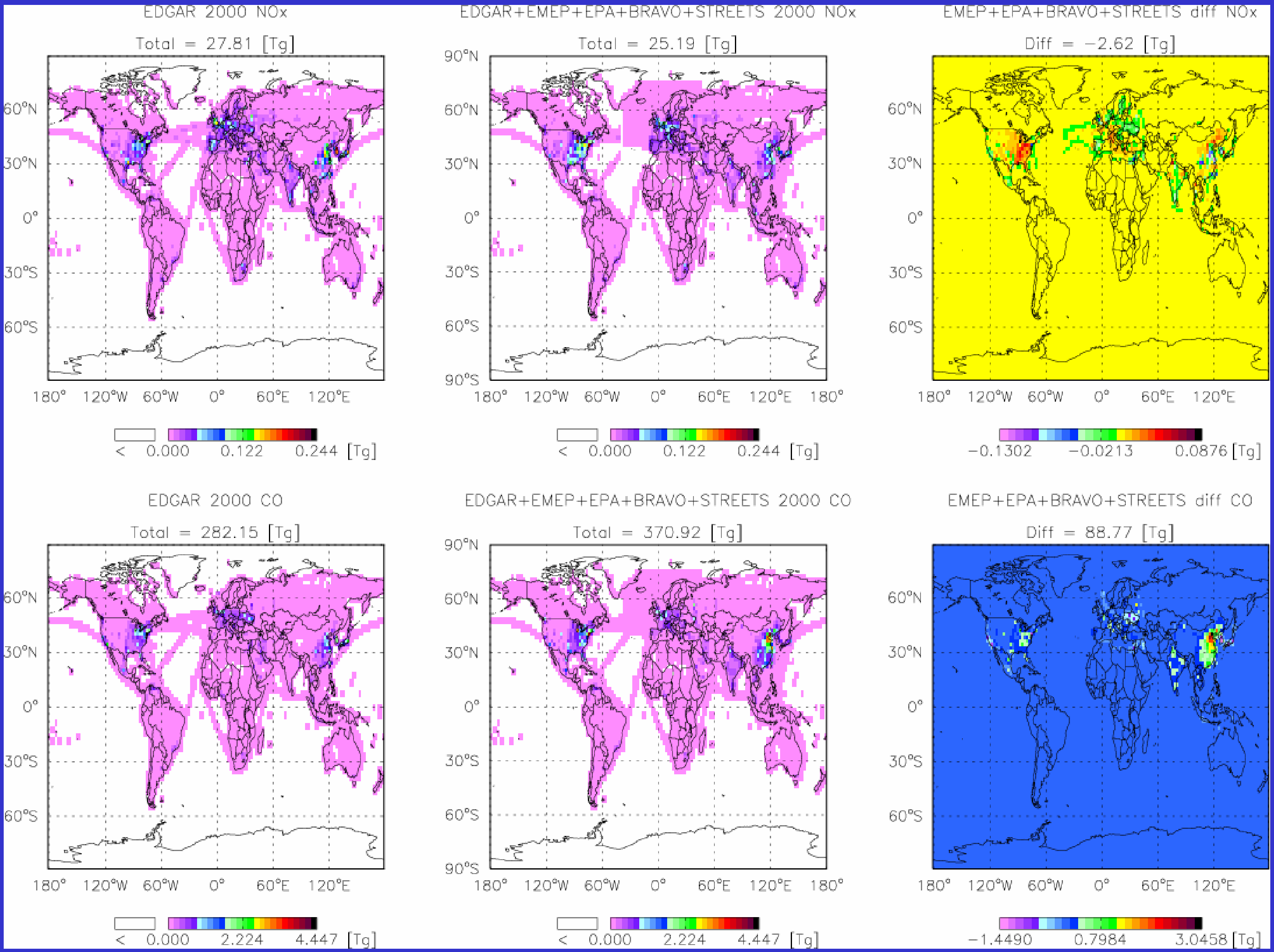
Default emissions (1995) vs. EDGAR

G-C species	Default	Uncorrected EDGAR	Corrected EDGAR	
NOx	23.6	27.8	25.2	Tg N
CO	402.5	282.1	370.9	Tg CO
SO2	60.3	67.4	56.3	Tg S
SO4	2.0	1.5	1.4	Tg S
NH3	40.6	40.6	46.3	Tg NH3
ALK4	24.2	24.2	19.9	Tg C
ACET	0.69	0.69	0.68	Tg C
MEK	0.80	0.80	0.48	Tg C
PRPE	8.0	8.0	6.9	Tg C
C3H8	10.1	10.1	10.0	Tg C
C2H6	6.8	6.8	6.0	Tg C

Default emissions vs. Corrected Edgar (2000)



EDGAR vs. corrected EDGAR (optional)



GFED2 Inventory for Biomass Burning

- This is now an option in GEOS-Chem
- 1997-2004 (2005 not yet in code but promised)

- Area burned from MODIS, 2001-2005;

  ATSR/VIRS, 1997-2000
- Fuel loads calculated from CASA model, driven by satellite data for NDVI
- Emission factors from Andreae and Merlet with updates

Van der Werf et al., ACP 6, 3423-3441, 2006.

Giglio et al., ACP 6, 957-974, 2006

GFED2 Emissions
CO, September
1997-2004